The Combined Chemical Dictionary on CD-ROM

USER MANUAL

Chapman & Hall/CRC Press
Electronic Publishing Division

Boca Raton London Washington DC

Published by Chapman & Hall/CRC, 2000 NW Corporate Blvd, Boca Raton, FL 33431 USA

CD-ROM

ISBN 0-412-82020-X

ISSN 1367-1952

User Manual

First edition 1997
Second edition 2000 (Version 4:1)

CAUTION

Treat all chemical substances as if they have dangerous properties. The publisher makes no representation, express or implied, with regard to the accuracy of the information contained in this Dictionary, and cannot accept any legal responsibility or liability for any errors or omissions that may be made.

The specific information in this publication on the hazardous and toxic properties of certain substances is included to alert the reader to possible dangers associated with the use of those compounds. The absence of such information should not however be taken as an indication of safety in use or misuse.

Contents

Technical support

For support on installation or use of the programs:

Technical Support Desk
Electronic Publishing Division
CRC Press LLC
2000 NW Corporate Boulevard
Boca Raton FL 33431 USA
Tel: 888-316-2367
Tel: 561-998-2562 (outside U.S.)
Fax: 561-998-9784
E-mail: techsupport@crcpress.com

If your query concerns your system set-up rather than problems with searching the database, please be prepared to supply the following information to the Technical Support Desk staff when you call:

- description of the problem, including any error messages displayed
- make and model of PC, including size of RAM and hard disk
- make and model of CD drive
- version of operating system and MSCDEX
- contents of CONFIG.SYS, AUTOEXEC.BAT, SYSTEM.INI and WIN.INI files
- display driver details under Display Settings in the Control Panel

For comments on the data or suggestions for inclusion, please contact:

The Editors, The Combined Chemical Dictionary
Chapman & Hall/CRC Press
Pocock House
235 Southwark Bridge Road
London SE1 6LY U.K.
Fax: 44 20 7407 7336
Email: enquiries@crcpress.com

Introduction

The Combined Chemical Dictionary on CD-ROM (CCD) is a chemical database containing over 456,000 substances which were formerly available from the following discs:-

Dictionary of Analytical Reagents (14,000 compounds)

Dictionary of Carbohydrates (22,000 compounds)

Dictionary of Inorganic and Organometallic Compounds (101,000 compounds)

Dictionary of Natural Products (156,000 compounds)

Dictionary of Organic Compounds (242,000 compounds)

PharmaSource (39,000 compounds)

The information contained on the chemical database includes descriptive and numerical data on chemical, physical and biological properties of compounds; systematic and common names of compounds; literature references; structure diagrams and their associated connection tables.

The CD-ROM contains a powerful search software from Hampden Data Services to provide text and structure searching. Previous experience with online searching, or with the use of CD-ROM products is unnecessary, although a basic familiarity with Microsoft Windows™ 95 is assumed.

Installation

Before you install ***The Combined Chemical Dictionary on CD-ROM*** check that you have the following recommended requirements for hardware and software:

Hardware

- Pentium II processor or higher
- 16 Mb RAM
- SVGA monitor
- 50Mb hard disc space
- Mouse
- 24x speed CD-ROM drive or faster

Software

- Microsoft Windows™ 95, 98 or NT 4.x

Installing the CD

Insert Disc 1 in the CD-drive and click on the **Start** icon and select **Run**

In the Command Line, type **D:\ccd\setup.exe** then click on **OK** or press Enter. (N.B. if your CD drive is other than D substitute the appropriate letter)

N.B. If you are a network user please see separate sheet for installation instructions.

Ensure that the Software box is checked. If you want a Combined Chemical Dictionary menu item to be added to your Start Menu, check the appropriate box.

N.B. You will need Adobe Acrobat Reader software to view the User Guide. If you do not already have a copy you may download it from the CD-ROM. To do this, click on ***Install Adobe Acrobat Reader*** *and follow the prompts. After installation of the Acrobat Reader you will need to run the* ***setup*** *program again.*

Type in the path to your CD-ROM drive and click on **OK**. You will now be prompted to select a folder in which to install the software. If you wish the programs to be installed into the **C:\hdsccd** folder just click on **Install CCD,** otherwise type in a new folder name before clicking on this button. You will then be prompted to insert Disc 2. Replace Disc 1 with Disc 2 and click **Continue**. Once complete a message will be displayed on-screen to indicate that the installation has been successful, unless you have opted for a hard disc installation.

Disc 2 contains all the chemical data for ***The Combined Chemical Dictionary on CD-ROM*** and so it is necessary to have this disc in the CD-drive in order to search the database.

Warning

All CD-ROMs from Chapman & Hall/CRC now incorporate a software clock. This means that your disc will cease to operate six months after its release date, when it should be replaced by the latest version.

Two on-screen warning messages will appear. The first indicates that the disc is about to expire and prompts you to install the latest version. The second message, several days later, is after expiry and no longer allows access to the old disc.

If at either of these warnings you have not received your new disc, please contact your distributor or Chapman & Hall/CRC as soon as possible.

In North and South America, Asia, Australia and New Zealand

CRC Press LLC

Electronic Publishing Division

2000 NW Corporate Blvd.

Boca Raton

FL 33431 U.S.A.

Tel: 888-318-2367

Tel: 561-998-2562 (outside U.S.)

Fax: 561-998-9784

E-mail: e-products@crcpress.com

In the UK, Europe, Middle East and Africa

CRC Press UK

Electronic Publishing Division

Pocock House

235 Southwark Bridge Road

London SE1 6LY U.K.

Tel: 44 20 7450 5083

Fax: 44 20 7407 7336

E-mail: enquiries@crcpress.com

Web site: http://www.crcpress.com

New features

- New streamlined interface enabling simultaneous text and structure searching
- 32-bit software, compatible with Windows NT
- Hit term highlighting
- Customisable report formats
- Directional searching
- Increased structure search speeds
- Structure Import/Export
- Viewable structures for variant and derivative compounds
- Viewing hit structures during structure search

Getting started

The Combined Chemical Dictionary on CD-ROM runs under the Microsoft Windows™ operating environment and is compatible with Microsoft Windows™ 95, 98 or NT.

Example of Structure & Text Searching

In the following example we will find all isocyanates which are reported to be toxic or lachrymatory. This involves a text search for all compounds which have the words TOXIC or LACHRYMATOR* in the text field, in conjunction with a structure search for N=C=O.

Run ***The Combined Chemical Dictionary on CD-ROM*** as described above, to display the Main Menu screen (Fig. 1)

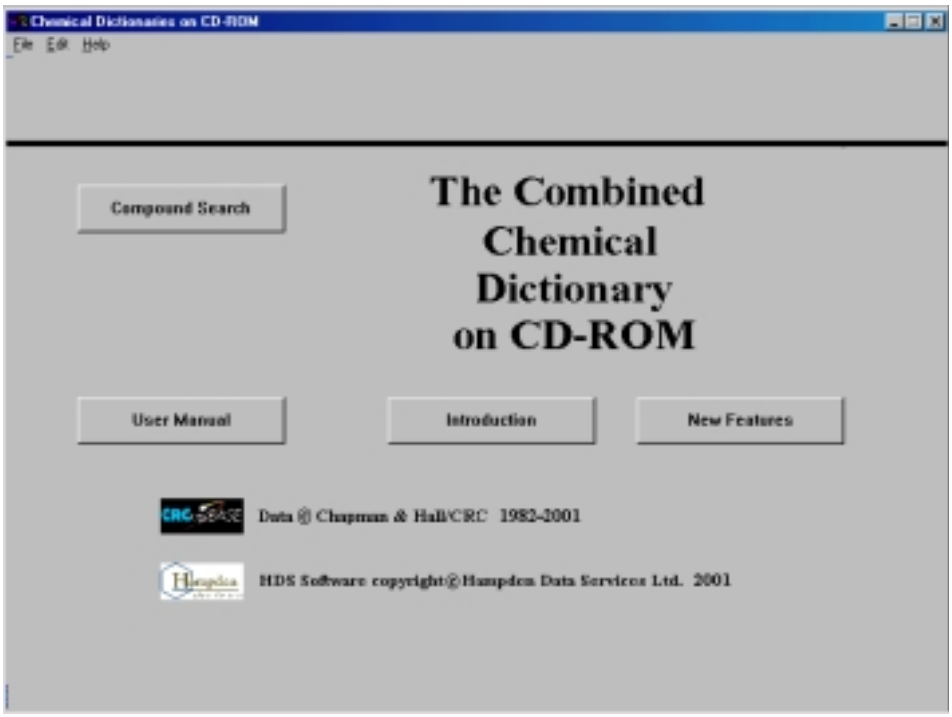


Fig. 1: Main Menu

Choose **Compound Search** to bring up the following screen:

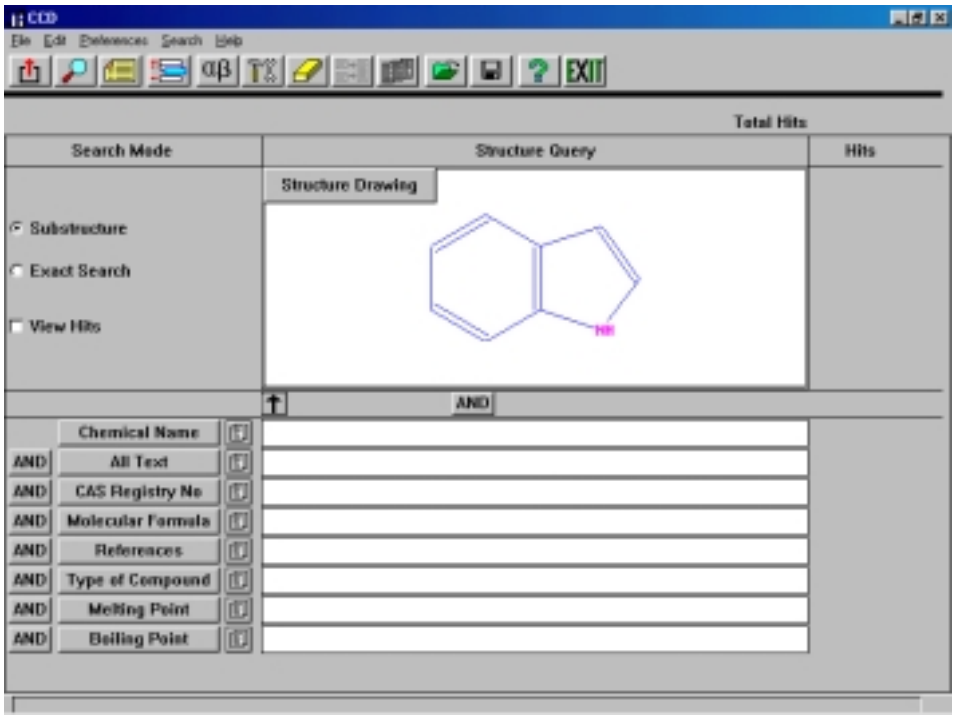


Fig.2: Compound Search Screen

Place the cursor in the **All Text** box, click on **Browse Index** icon  to display the **All Text** index:

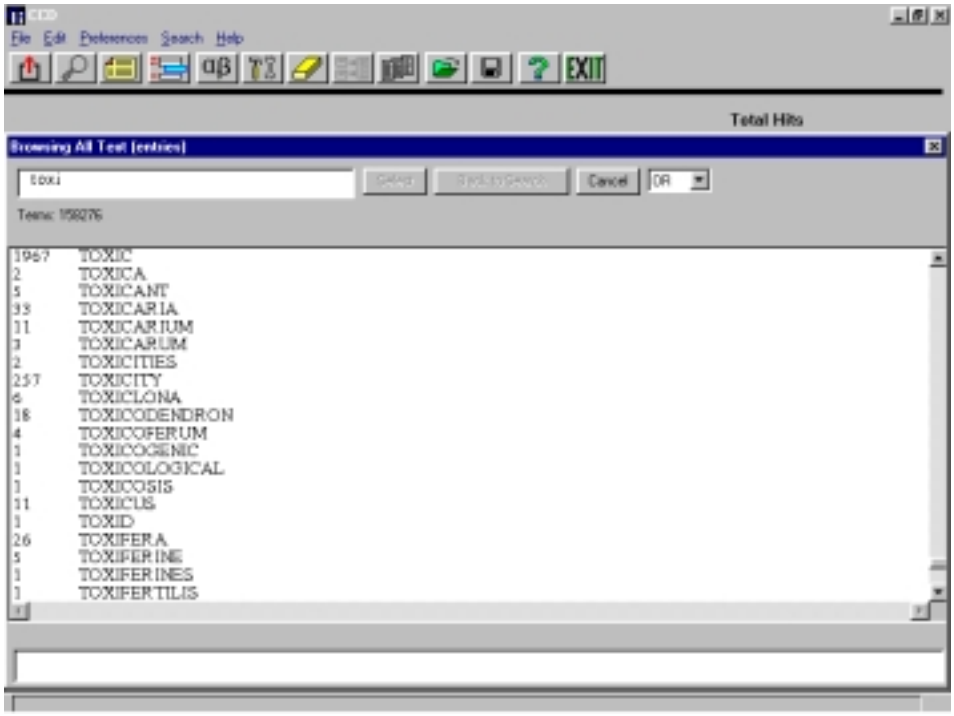


Fig.3: Browse All Text Index

Start typing **toxic** and the index will move downwards. To transfer the highlighted index term to the search box, highlight the required term and click on **Select** (alternatively double click on the required term) followed by **Back to Search**. You can also enter the search terms without using the index by typing directly into the **All Text** search box.

To extend the search to **TOXIC** or **LACHRYMATOR***, in the **All Text** search box, click the cursor after the word **TOXIC** and then click on the **Operator Toolbox** icon  in the tool bar (N.B. If the Operator

Toolbox is obscuring any part of the screen you can move it: position the cursor in the title bar at the top of the toolbox, press and hold down the mouse button, then drag the cursor to another position on the screen). Position the cursor on **OR**, then press the mouse button. The word **OR** is transferred to the **All Text** search term box. You can close the Operator Toolbox by clicking the **X** in the top right-hand corner. Now, type in the search term: **LACHRYMATOR***

Your complete **All Text** search term should now be: **TOXIC OR LACHRYMATOR***

Now you can prepare the structure query. First click on **Structure Drawing** button to bring up the Structure Drawing screen. The structure drawing tools are shown on the left-hand side of the screen, and the **Pencil Tool**, at the top, is highlighted. This is used for drawing and modifying individual atoms and bonds.

To draw the isocyanate group, start by drawing a chain of 3-carbon chain as follows:

Click on the **Chain Tool**  . A dialog box is displayed giving a default chain length of 1. Press the backspace key, then type in the number 3. Click on **OK**. The cursor changes to a chain. Position the cursor in the centre of the screen and click the mouse to draw a 3-carbon chain.

To modify the chain, click on the **Pencil Tool**  (the cursor changes to a pencil).

Modifying the atoms: To select a nitrogen atom, change the **Current Atom** (displayed in the bottom left-hand box) to nitrogen by clicking on "N" in the atom/bond palette. Position the point of the pencil over the node to be changed (an "A" will appear on the pencil when correctly positioned over an atom) and click. Repeat this procedure for the right-hand node, using oxygen from the atom/bond template.

Modifying the bonds: Change the **Current Bond** value to double by double clicking on the double bond box on the right-hand side of the atom/bond palette. Position the point of the pencil over one of the bonds to be changed (a bond will appear on the pencil when correctly positioned over the bond) and click. Repeat this procedure for the second bond.

If you make a mistake when structure drawing, you can:

1. Clear the drawing screen completely: click on **File**, then **New**.
2. Delete the last action: click on **Edit**, followed by **Undo**.
3. Click on the **Eraser Tool**  . To erase an atom, position the end of the eraser over the atom, then click the mouse. To erase a bond, position the end of the eraser over the centre of the bond, then click.

Query definition

When you have drawn the structure, you must define the specific attributes required when you use the structure as a query. For example, do you want the chain bonds you have drawn to occur only as chain bonds in the file structures, or could they be part of another ring system?

As you are searching specifically for an isocyanate functional group, the chain bonds and nodes should not be part of another ring system and the chain bonds should match exactly. If you do not carry out any query definition, the default values for query definition will apply and many of the retrieved structures will not be relevant. For example, in this case you will retrieve structures with amide groups (since the default bond values are exact/normalised).

Before using the query definition options, you must first select the bonds. Click on the **Selection Tool**  , and the cursor changes to a box shape.

Defining the bond characteristics: Position the centre of the cursor box over the centre of one of the chain bonds, and click the mouse button to highlight the bond. Hold down the shift key and position the cursor over the other chain bond and click (if you do not hold down the shift key, you can only select one bond). Both chain bonds will now be highlighted. Click on the **QueryDef** menu, followed by **Bond Characteristics**. Click on **Exact** under Bond Value, then click on **OK**.

Query verification

You must now verify that you have defined the correct attributes for the atoms and the bonds. Click on the **QueryDef** menu again, then click on **Query Verification**. Click on **OK** to verify all the bonds, nodes and rings (where present in your structure query). Each type of bond, node and ring will be highlighted in turn, where appropriate, and details of the attributes are given at the bottom of the screen. Click on **OK** each time to move on to the next box. If you have made any mistakes, go back to the query definition again and repeat that stage.

When you have completed your structure query click on the GREEN ARROW in the Structure Drawing Screen to transfer the query to the Compound Search screen.

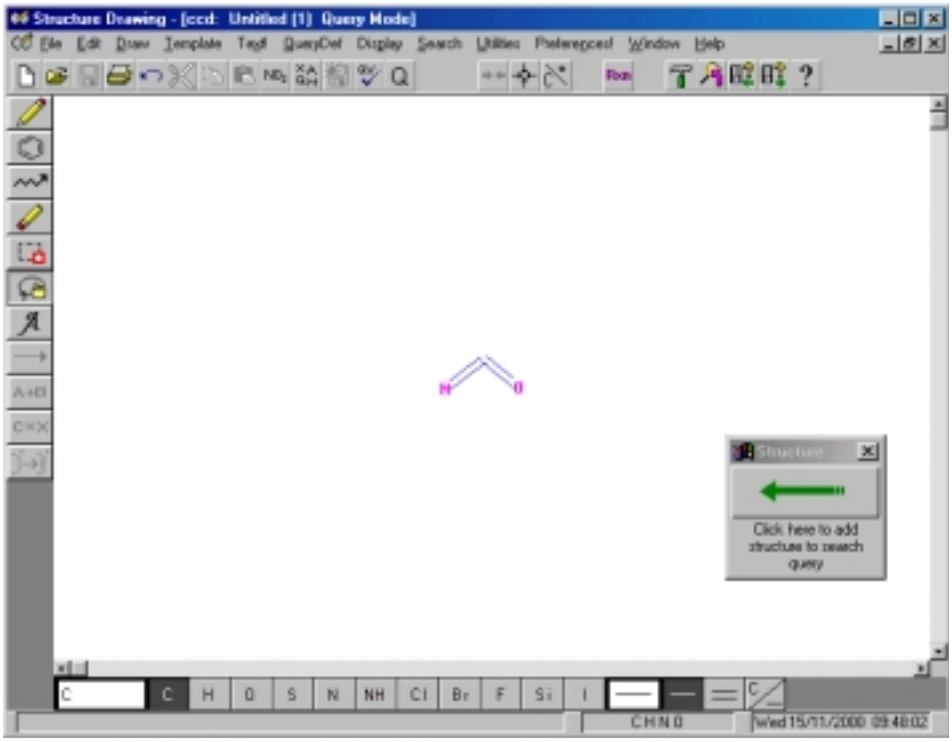


Fig.4: Structure Drawing Screen

Starting the search

Ensure that the Boolean operator between the structure search box and the text search fields is set to **AND**. If not simply click on it to toggle through the available operators (AND, OR, NOT).

You may choose the order in which text and structure searches are performed. The order is indicated by the direction of the arrow linking the structure search and the text search boxes. Generally **the total search time is shorter if the text search is performed first** as the structure search is then carried out only on the text search results and not on the whole database. The default is text first, and this is indicated by the upward arrow  . Should you wish to perform the structure search first, simply click on this button to change the arrow direction downwards. To view the hit structures during the structure search, select **View Hits**.

Click on the **Run Search** icon  on the menu bar at the top of the screen. The number of hits obtained will be shown at the top of the screen.

To view the hits, choose the **Hitlist** icon  from the menu bar. To view any record simply double click on it. All occurrences of the search term are highlighted.

To print the hitlist from a search, select **Print Hit List** in the File Menu and you will be prompted to choose All Rows, Current Row or a range of rows. Select the appropriate print option and click **OK**.

To print the hits from the summary list as complete entries, click on the **Print** icon  . You will then be prompted to choose between printing the current record, or all records.

You can also print out the hitlist as a customised report format containing whichever fields you choose, and in whatever order. Click on the **Report Settings** icon  to display a list of all available fields. See section **Viewing and Printing Search Results** for more details.

You can bookmark or unmark items by clicking on the **Bookmark** icon  .

Entries may also be transferred to the clipboard for export, for example to word processing packages.

To copy the entry to the clipboard, click on the **Edit** menu and choose **Select All**. To copy the text, choose **Copy Text** from the **Edit** menu. To copy the diagram, choose **Copy Image** from the **Edit** menu.

Note that you must switch on the structure display, by clicking on the structure icon  , in order for **Copy Image** to become active.

To return to the Compound Search screen, click on the **Back** icon  from the menu bar.

Text and data searching

Entering the search term

You can search any of the fields listed. Each field contains an index of all the terms in that field – to display the index, click on the **Browse Index** icon  . You can enter search terms using the index, or type the terms directly into the Search Terms box, using truncation to enter long chemical names. For a description of the content of individual fields, use the electronic **Help** screens.

Selecting the search term using the Index

1. Type the first part of the required search term in the **Index Stem** box (you may need to press the Backspace key to remove the first entry). The correct part of the index will then be displayed. Continue to type the search term until the required term is displayed in the index.
2. Highlight the required search term and click on **Select** to transfer the search term to the search box (alternatively double click on the required search term). Additional search terms may be added by repeating step 1 (see below for Combining Search Terms).
3. If you do not want to add any more search terms, click on **Back to Search.**

You can enter search terms into as many of the search fields as you wish (see below for Linking the Fields in the Search).

To carry out the search click on the **Run Search** icon  .

Go to page 28 for instructions on examining the search results.

Available fields to search

You can choose from 22 text and data fields to search. The default search screen lists 8 fields (All Text, Boiling Point, CAS Registry Number, Chemical Name, Melting Point, Molecular Formula, References, Type of Compound) but you can add or delete fields as you like (see section below for details). For a description of the individual field contents view the electronic **Help** screens.

All Text	Ion Charge
All Entries	Melting Point
Boiling Point	Molecular Formula
Boiling Point Pressure	Molecular Weight
CAS Registry Number	Optical Rotation
Chemical Name	Partition Coefficient (Calc.)
Density	References
Dictionary Subset	RTECS Accession Number
Dissociation Constant	Supplier
Hazard and Toxicity	Type of Compound
Hazard Flag	Type of Compound Words

Combining search terms

You can link the search terms using combinations of **AND**, **OR**, **NOT**, and you can use search relations, such as >, < = when you are searching for numerical data.

All the available options and other search relations are in the Operator Toolbox accessed by clicking on the **Toolbox** icon: 

Examples of combining search terms

AND

To find all compounds which have antiparkinsonian and antidepressant properties enter the following search in the **Type of Compound Words** field:

antiparkinsonian and antidepressant*

To search for all compounds that contain $C_{30}H_{36}$ as part of their molecular formula, enter the following search terms in the **Molecular Formula** field:

C30 AND H36

OR

To find all compounds which have been isolated from either a root or fruit, enter the following truncated search terms in the **All Text** field:

root* or fruit*

NOT

To exclude ALKALOIDS from this search, enter:

root* or fruit* not alkaloid*

RANGE SEARCH

To search for all compounds with a boiling point between 100^{o} and 105^{o}, enter the following search terms in the **Boiling Point** field:

100 - 105

N.B. For range searching use the Range Operator from the Operator Toolbox. Alternatively, you can use a hyphen but you must remember to insert a space between hyphen and numbers.

NEGATIVE NUMBERS

To search for all compounds with a melting point between -5^{o} and 5^{o}, enter the following search terms:

-5 - 5

To add, delete or change a field in the list of search fields

Click on the **Edit Search Form** icon  to display the following dialog box:

Fig. 5: Edit Search Form

- **Adding** a field – From the right-hand box, select the field you want to add to the search form. Click on **Insert Item**. If you want to make this the default search form check the **Save As Default** box, then click on **Save**. You will be prompted to provide a filename for this new search form. Click on **OK**.
- **Deleting** a field – From the left-hand box, select the field you wish to remove. Click on **Delete Item.**

- **Changing** the default search form – Select all the fields you wish to include, check the **Save As Default** box, then click on **Save**. You will be prompted to provide a filename for this new search form. Click on **OK**.
- To show all 22 fields – click on **All Fields** then click on **OK**.

Linking the fields in the search

You can change the option on the button to the left of the search field. Click on the button to toggle between **AND**, **OR** and **NOT**. You can also combine search terms within a field using the **Operator Toolbox**.

Sample Search

To find all terpenoid compounds that have been isolated from the genus *Taxus*, enter the search terms as follows:

	All text	taxus
AND	All Entries	
AND	Chemical Name	
AND	Molecular Formula	
AND	Type of Compound	
AND	Type of Compound Words	terpenoids

If you are performing a structure search in combination with a text search you can change the Boolean operator linking the text and structure search boxes by clicking on it and toggling between the options.

Special symbols

The Special Symbol keypad contains all the Greek characters and other symbols you may need when entering a search term. You can access this by clicking on the icon: 

Truncation and wild cards

Use the following characters as wildcards and for truncation:

- ***** to indicate a string of characters – either within the search term, or at either end of the term, to truncate the term
- **?** to indicate a single letter within a word

You can use a combination of * and ? within a search term.

If you use an * at the end of the search term to truncate the term, it will save entering all the possible variations of the search term. For example, if you search for **HORMON*** in the **All Text** field, you will retrieve all compounds which are **HORMONES**, **HORMONAL**, **HORMONE-DEPENDENT**, **HORMONE-RELEASING** etc.

Using left-hand truncation, you can search for classes of compounds. For example, a search for ***TOXIN** in the **Chemical Name** field will retrieve all compounds whose names end in TOXIN, such as **AMPHITOXIN**, **BREVETOXIN B**, **WIKSTROTOXIN A** etc.

Structure searching

You can use a structure search on its own, or in combination with a text search.

To prepare a structure search, you must:

- draw the structure, as described in the section on drawing and editing structures (page 18)
- prepare the structure query, for an exact match or for a sub-structure search, as described in the section on preparing the structure query (page 24).
- **transfer your query to the Compound search screen by clicking on the GREEN ARROW**

For further details about all the options in structure searching, consult the electronic **Help** screens.

The Structure Drawing screen

Click on the **Structure Drawing** button in the Compound Search Screen to display the Structure Drawing screen:

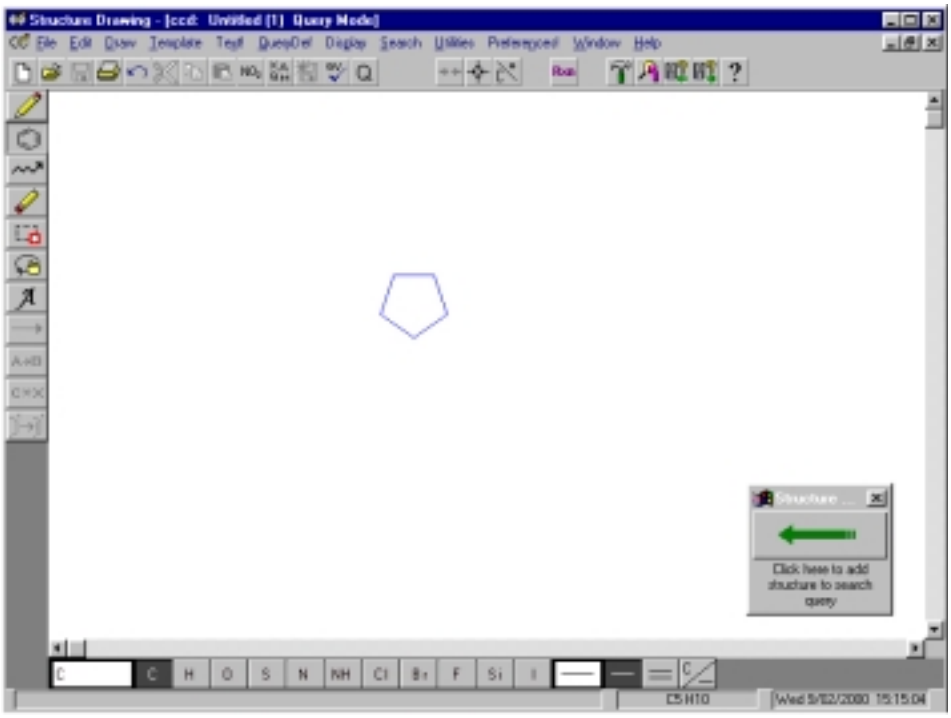


Fig. 6: The Structure Drawing screen

The structure drawing screen consists of:

- a **drawing palette** containing tools for drawing structures (left-hand side of screen)
- a **Common Atoms** and **Common Bonds palette** (bottom of screen)
- a **Toolbar** (optional) to display buttons for frequently used commands. This can be switched on and off using the Layout option in the Preferences menu. The icons in the toolbar are explained on page 35.
- a **title bar** at the top of the screen
- a **menu bar** with options for drawing, filing, editing, searching and displaying structures
- a **green arrow** to transfer your query to the Compound Search screen

Drawing structures

You can draw structures by:

- using the drawing tools
- calling up a template for editing

The drawing tools

Pencil Tool

Ring Tool

Chain Tool

Eraser Tool

Selection Tool

Lasso Tool

Text Tool

Reaction Arrow Tool - *not used in this application*

Reaction Role Tool - *not used in this application*

Reaction Site - *not used in this application*

Reaction Mapping Tool - *not used in this application*

To draw a structure, use the Pencil Tool, the Ring Tool or the Chain Tool. Select the required tool, then move the cursor to where you want the object, and click the mouse button. The atoms and bonds drawn will be the Current Atom and Current Bond, which are shown in black-bordered rectangular boxes at the bottom of the screen. See next section for details of drawing and modifying atoms and bonds.

Pencil Tool

Use the Pencil Tool to draw atoms and bonds. To draw two nodes connected by a bond, position the cursor where you want the first node to be placed. Press and hold the mouse button down, whilst you drag the cursor to the point where you want the second node to appear, then release the mouse button. The atoms and bond drawn will be the Current Atom and Current Bond (see previous section).

Modifying atoms and bonds using the Pencil Tool

Use the Pencil Tool for changing atoms or bonds in the Structure, unless you wish to modify a large number of atoms or bonds, when you should use the Selection Tool.

When the Pencil Tool is correctly positioned over a bond, a small line will appear along the middle of the pencil. Similarly, a small “A” will appear when the pencil is correctly positioned over an atom.

Modifying bonds: If the Current Bond is single, you can draw a double bond by “drawing” another bond over an existing bond: drag the pencil Tool from one node to the other, retracing the existing bond (convert from a double bond to a triple bond in the same way). You can also modify an existing bond by first changing the Current Bond: choose a new bond value from the palette at the bottom of the screen, or from the Bond menu. If you make a single click on the new bond value, it makes a temporary change to the Current Bond (after one use, it reverts to the previous value); whereas a double click on the new bond value makes a permanent change. When you have selected the new bond, place the tip of the cursor on the middle of the bond to be changed and click. The bond will then change to reflect the new Current Bond. (To return the Current Bond to Single, press the Space Bar).

Modifying atoms: First change the Current Atom to the required symbol, by selecting one of the common atoms at the bottom of the screen, or using the Atom menu (again, a single click on the new atom makes a temporary change and a double click makes a permanent change). Place the tip of the pencil cursor over the node to be changed and click. The node will change to reflect the Current Atom (To return the Current Atom to Carbon, press the space bar).

Ring Tool

Use the Ring Tool to draw 3- to 15-membered rings. Select the Ring Tool, then type in the ring size, or select one of the pre-defined ring types displayed, and click on **OK**. Position the cursor where you want to draw the ring on the screen, and click. You may continue to use the selected tool to draw similar rings. To draw a spiro ring, position the cursor over an existing ring node and click. The second ring will be spiro fused to the first. To draw a fused ring, position the cursor in the middle of an existing ring bond, and click. The second ring will be fused to the first along the selected bond. Fused ring systems can be drawn using the Feldmann notation, details of which are given in the electronic **Help** screens.

Chain Tool

Use the Chain Tool to draw chains of length 1 to 30 nodes. Select the Chain Tool, then type in the length of the chain you require. The default is 1. Click on **OK**. Position the cursor where you want the chain to start (either over an existing node, or in a space on the screen) and click. A chain, of the length specified, is drawn in a logical way.

Eraser Tool

Use the Eraser Tool to delete an atom or a bond. Click on the Eraser Tool. To erase an atom, position the tip of the cursor over a node and click. To erase a bond, position the tip of the cursor over the middle of the bond and click.

Selection Tool

Use the Selection Tool to highlight nodes and bonds, before deleting or modifying them, or prior to query definition (see page 24). Click on the Selection Tool and the cursor changes to a rectangle containing a cross. Select items as follows:

a node	position centre of cursor over node and click*
a bond	position centre of cursor over centre of bond and click*
part or all of a structure	draw a rectangle round the structure: position the cursor at the top left hand corner of the rectangle, press and hold the mouse button, then drag the mouse button down across the structure to draw a dotted rectangle encompassing the required group of atoms. Release the mouse button. To deselect one of the selected nodes, position the cursor over the node, press and hold the Shift key and click.

* To select more than one disconnected node or bond, press and hold the Shift key whilst selecting the nodes or bonds.

Lasso Tool

Use the Lasso Tool to select a structure if you want to move it to another location on the screen. When you select the Lasso Tool, the cursor changes to a lasso. Press and hold the mouse button as you drag the cursor round the object to be moved. Release the mouse button, then move the cursor inside the lassoed area. The cursor changes to a hand. Press and hold the mouse button and drag the hand to the new position on the screen. Release the mouse button. To remove the currently drawn lasso, click outside the lasso.

Other tools in the palette

Use of the Text Tool is described in the electronic **Help** screens. Reaction searching is not available on this CD-ROM.

The Draw menu

The Draw menu allows you to select bonds, atoms, shortcut symbols and variable atoms, and to fuse fragments together. Brief details of the use of the Bond, Atom and Shortcut options are given below. For details of the other options, see the electronic **Help** screens.

Bond

Use the Bond option in the Draw menu to select a new Current Bond value. A box is displayed giving all the possible bond types. Click on the required bond type, then click on **Single Use** or **Multiple Use** according to whether you wish to make a temporary change or a permanent change to the Current Bond.

Atom

Use the atom option in the Draw menu to select a new Current Atom. A box listing all the available atoms is displayed, with the common atoms down the left-hand side and the rest of the atoms in alphabetical order. Click on the required atom, then click on **Single Use** or **Multiple Use** according to whether you wish to make a temporary change or a permanent change to the Current Atom. In Query Mode, there is also an option to exclude the selected atom from the search query. Click on **Exclude** and when you draw that atom on the screen, it will appear underlined.

Shortcut

The Shortcuts are predefined common groups of atoms, usually with one point of attachment. You can select a Shortcut in the same way as you select an atom (see above). Some Shortcuts can be drawn in the reverse direction (those that can be reversed are marked with a small square next to the selection button). To reverse the display of the shortcut, highlight the shortcut, then use the **Reverse Shortcut** option in the **Display** menu.

The Display menu

The options in this menu allow you to change the display of the structure on the screen. Brief details of the options are given in the table below. For further details, see the electronic **Help** screens.

Carbons	Use this to change the display of pre-selected carbon atoms from **Angle** mode to **Dot** mode or to displaying **C** symbols
Show Hydrogens	Displays hydrogens on terminal carbons and heteroatoms with spare valencies
Show VPA	If you have defined an atom with a variable point of attachment, use this option to show all the potential sites of attachment
Show Node Numbers	Inserts node numbers on every atom in the structure
Show Reactions	Shows the role, (e.g. reactant, or product) of each compound in the reaction. *Not used in this application*
Smooth	Use this to straighten and align structures that have been drawn freehand
Expand	Enlarges and centres the drawing on the screen
Contract	Contracts and centres the drawing on the screen
Reverse Shortcut	Reverses the display of Shortcut symbols (where available)
Rotate	Rotates a structure about an atom. Pre-select the structure first
Flip fragment horizontal	Use this to flip the structure from left to right or vice versa
Flip fragment vertical	Use this to flip the structure from top to bottom or vice versa
Snap to Grid	Displays a grid on the screen – where possible, bonds are moved to align with the grid lines. To remove the grid lines, click on Drawing in the Preferences menu, then click on Grid
Snap to Compass	Aligns a pre-selected set of nodes to the nearest compass position

Using Templates: the Template menu

Template files are files of structural fragments, which you may use when drawing your structure. You can add new templates, which contain fragments that you use frequently. You should create a separate sub-directory to contain your own template files.

Open

Click on **Open** to open a template file. A box is displayed giving the list of template files available (or change the directory to locate template files that you have created). Use the mouse to scroll down the list of templates, then click on the template file that you want. The structures in the template will be displayed in the small window. If they are the required structures, click on **Open**.

The fragments in the template file are displayed. Click on a node or bond in the fragment you require, then click on **OK**. You are returned to the drawing window and the cursor changes to a Fusion cursor. Click on a free space to draw the template on its own, or, if you have selected a bond in the template, you can fuse the template structure on to an existing structure by clicking on a bond of the existing structure. For a spiro fusion, you must click on an atom in the template structure and an atom in the existing structure. You will get a warning if the valency of an atom will be exceeded as a result of the fusion.

Edit

Select **Edit** from the Template menu, if you want to modify a template file. Open the required template file, as described above, then you can draw any additional template structures, or editing any of the templates displayed. When you have finished editing the structures, select **Save** to store the structures.

Save

Select **Save** to save the structures currently drawn on the screen as a template. You may change the name of the file in which the templates are stored.

Editing structures: the Edit menu

The Edit menu provides standard editing commands, such as Cut, Copy and Paste. Brief details of the options are given in the table below. For full details, consult the electronic **Help** screens. Before using the Cut, Copy or Clear commands, you must pre-select the object(s) first in one of the following ways:

- use **Select All** from the **Edit** menu
- highlight a specific node or bond using the **Selection Tool**
- use the **Selection Tool**, or the **Lasso Tool**, to draw a rectangle or loop round the required atoms and bonds.

Undo	Use this to undo the last action made
Cut	Deletes the selected objects and places them on the Clipboard
Copy	Copies selected objects to the Clipboard
Paste	Pastes objects from the Clipboard into the current structure drawing window
Select All	Selects all the items on the screen
Clear	Deletes selected items from the screen
Clear All	Clears the whole screen
Show Clipboard	Displays the contents of the Clipboard
Repaint	Updates the display on the screen
Delete Mappings	*Not used in this application*

Filing and printing structures: the File menu

The File Menu provides commands for opening new and existing files, saving and printing. You can use the options in the File menu to prepare your own structure collections. When preparing structure queries you must use **Query Mode**. If you just want to draw and print structures, use **Structure Mode**. Select the **Change Mode** option in the QueryDef menu to change to Structure Mode.

Brief details of the options in the File Menu are given in the table below. For full instructions consult the electronic **Help** screens.

New	Clears the drawing screen ready to draw a new structure
Import	Use this option to import structures
Export	Use this option to export structures
Save	Saves structure currently displayed on the screen
Save As	Saves displayed structure under a new name
Page Setup	Allows you to set options relating to printing the structure, e.g. page size
Print	Prints the structure currently displayed
Exit	Returns you to the Compound Search screen

Structure Import/Export

The Import/Export facility within the structure drawing screen allows a connection table for a given compound on the database to be saved to disk or transferred to or from another drawing package.

Import

The structure formats available for importing structures are SMD (.SMD), DARC F1 (.DRC), MOLFILE and Alchemy (both .MOL) and the structures are stored with one structure per file.

To import a structure, click on the **File** menu within the structure drawing screen and select **Import**. The **Import dialog box** (Fig.7) will appear on-screen allowing the choice of the appropriate structure file format.

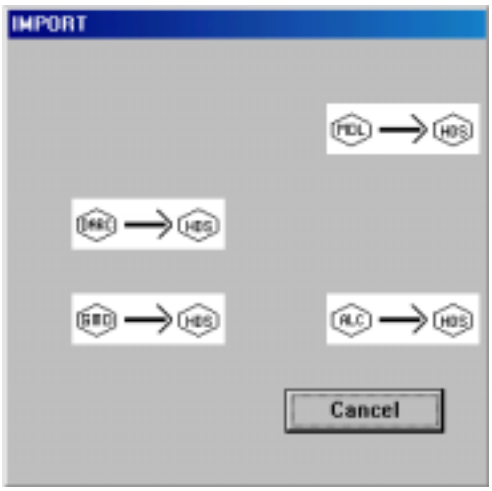
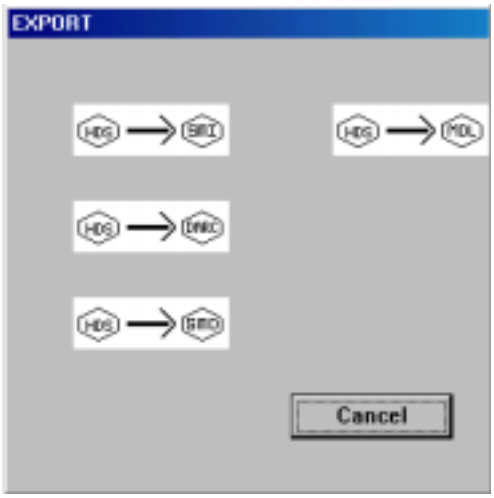


Fig.7: Import dialog box

Select a format and a second dialog box will appear. Locate the desired structure file via selecting the appropriate drive letter and use of [..] tool. Once located select the desired filename and click **Open**. As a result the structure will be imported and displayed on-screen as a connection table.

Export

The structure formats available for exporting structures are SMD (.SMD), DARC F1 (.DRC), MOLFILE (.MOL) and SMILES (.SMI) and the structures are stored with one structure per file. As the structures are exported as queries, normalised and exact/normalised bonds become unspecified in the MOLFILE.
To export a structure, click on the **File** menu within the structure drawing screen and select **Export**. The **Export dialog box** (Fig.8) will appear on-screen allowing the choice of the appropriate structure file format.
Fig.8: Export dialog box



Select a format and a second dialog box will appear. Locate the desired directory to where the diagram is to be exported via selecting the appropriate drive letter and use of [..] tool, provide a filename and click **Open**. As a result the structure will be exported as a connection table.

Preparing the structure query

When you have drawn the structure query, use the options in the QueryDef menu to define the precise attributes for your query. If you do not define any attributes, the defaults will apply (see page 25).

To set an attribute, you must first pre-select the required node(s), bond(s) or ring, using the Selection Tool  , then choose the appropriate command from the QueryDef menu: **Ring Isolation**, **Bond Characteristics**, **Node Characteristics**.

Note If you select a mixture of ring nodes, bonds and chain nodes, you will not be able to proceed with query definition.

The QueryDef menu

A summary of the options in the QueryDef menu is given below. For further details consult the electronic **Help** screens.

Change Mode

To prepare structure queries, you should be in Query Mode (the mode is indicated at the top of the screen). Click on **Change Mode** to change to Structure Mode only if you want to create your own files of structures.

Ring Isolation

This option is active only if you have selected one or more nodes in a ring. Select an Isolated ring if you want the query ring system to exactly match the ring system in the retrieved structures. Choose Isolated/Embedded if you do not mind if the query structure is embedded within a larger ring system

Bond Characteristics

Select one or more bonds of the same type (e.g. all bonds in ring, or all carbon-carbon chain bonds). If you select ring bonds, you cannot change the bond type. If you select chain bonds, you can choose whether you want the bonds to occur in a chain, a ring or either, when you search. You can choose the Bond value to be Exact, Normalised. Exact/Normalised or Unspecified.

Node Characteristics

You cannot change the definition of a ring node. Pre-select a chain node or nodes. You can then choose whether the selected nodes should occur in a chain, or in a ring, or either, when the search is carried out.

Hydrogen Attachments

Use this option to define the number of hydrogen atoms attached to a given node. Pre-select the required node. Under **Hydrogen Attachments** click on **Specific** followed by **Exact** or **Minimum** and type in the number.

Non-Hydrogen Attachments

Pre-select a node, then click on **Non-Hydrogen Attachments** to define the number of atoms, other than hydrogen, connected to a given atom.

Other Attributes

To use this command, you must first pre-select a node. You can then select **Other Attributes** to change the Charge, Valency or Isotope values on a node.

Delocalised Charge

Pre-select a group of nodes, then select **Delocalised Charge** to specify the required charge over the selected nodes.

Query Verification

When you have defined all the attributes required for your search, click on **Query Verification**, to review the definitions of your query. Click on **All** to view every feature, or click on **Select** then click on the specific features you want to view. Each feature is then displayed in turn, for you to click on **OK**, or **Cancel**. If you select cancel at any time, the highlighted nodes or bonds are automatically pre-selected when you return to the editing screen.

Printing out the query structure. Before starting the search, you can print out your query structure together with all the defined attributes. Select the **File** menu, click on **Print** and then **OK** (alternatively, click on the print icon in the Toolbar).

To print out only specific items from within the print box, e.g, **Print Attributes**, deselect the unwanted items and click **OK**.

Query definition defaults

You can carry out a search ***without*** defining any attributes and the following defaults will apply:

- all nodes and bonds drawn in a chain in the query structure must occur in a chain in the database structure to satisfy the search query
- all nodes and bonds drawn in a ring must occur in a ring
- all rings in the query structure are set to being isolated/embedded (i.e. rings embedded within a larger ring system will be retrieved)
- alternating single and double bonds in an even-membered ring path are normalised
- tautomeric sequences (according to CAS conventions) are normalised
- all bonds in isolated/embedded rings are set to exact/normalised
- bonds between carbon atoms in isolated rings are set to exact
- bonds between heteroatoms (or between a carbon and a heteroatom) in isolated rings are set to exact/normalised
- chain bonds between carbon atoms are set to exact
- chain bonds between heteroatoms or carbon-heteroatom bonds are set to exact/normalised, except the following, which are set to exact:

  when an oxygen has two bonds to it, neither of which are H, D or T;

  R–X bonds, where X is a halogen and R is not N, S, Se, Te or O

N.B. The above defaults apply only if you are in Query mode. You can carry out a search if you are in Structure mode, but different defaults apply and you cannot change them.

If you want to change the default values and set your own attributes to define your query, most of the default attributes can be changed.

You can request that rings must be isolated. Chain bond values can be set as Exact or Normalised, or either, or unspecified. Chain nodes can be set as Chain or Ring or either.

Searching the database

Text only search

After you have entered the search terms, check that all Boolean operators between different fields are set as required (to change an operator simply click on the operator button until you reach the correct one). Then click on the **Run Search** icon  .

Structure only search

After you have drawn your query and transferred it to the Compound Search screen, choose either **Exact Search** or **Substructure Search** by clicking the appropriate radio button. To view the hit structures during the structure search, select **View Hits**. Then click on the **Run Search** icon  icon.

Text and structure search

After you have prepared your search query, ensure that the Boolean operator between the structure search box and the text search fields is set as required (the default is **AND**). If not simply toggle through the available operators (AND, OR, NOT).

You may choose the order in which text and structure searches are performed. The order is indicated by the direction of the arrow linking the structure search and text search boxes. Generally **the total search time will be shorter if the text search is performed first** as the structure search is then carried out only on the text search results and not on the whole database. The default is text first, and this is indicated by the upwards arrow  . Should you wish to perform the structure search first, simply click on this button to change the arrow direction to downwards. To view the hit structures during the structure search, select **View Hits**. Then click on the **Run Search** icon  .

The number of hits obtained is displayed at the top of the screen. To view the hitlist, click on the **View Hitlist** icon  . See below for instructions on analysing the search results.

Combining hitlists

Hitlists from the current search session may be combined by using the Boolean operators **AND**, **OR** and **NOT**. Click on the **Combine Hitsets** icon  :

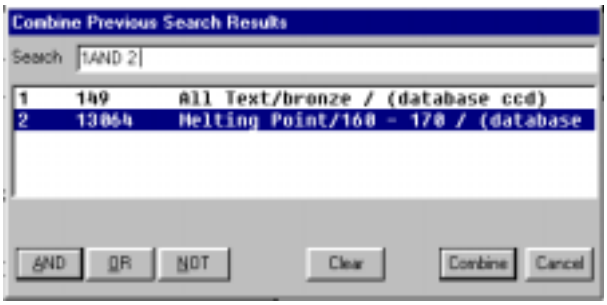


Fig. 9: Combine hitlists

If, for example you wanted to find all entries present in both searches 1 and 2 - you would select search 1, click on the **AND** operator, then select search 2, then click on **Combine**. The resulting hitlist is then saved as the next search number, and can be viewed by clicking on the **Show Search History** icon  :

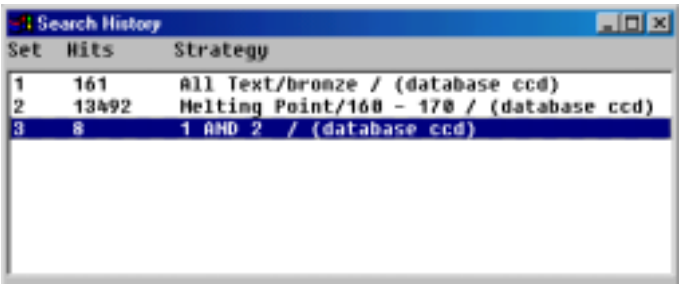


Fig. 10: Show Search History

Simply select the desired hitlist, then click on the **View Hitlists** icon  to view the results.

Saving and retrieving queries

If you wish to save a search query simply click on the **Save Strategy** icon  and choose a filename.

To retrieve a saved search query click on the **Open Strategy** icon  , select the required query and click on **OK**. Note that it is the query that is saved, not the hitlist itself.

Viewing and printing search results

Click on the **View Hitlists** icon  to view the search results as shown in Fig.11

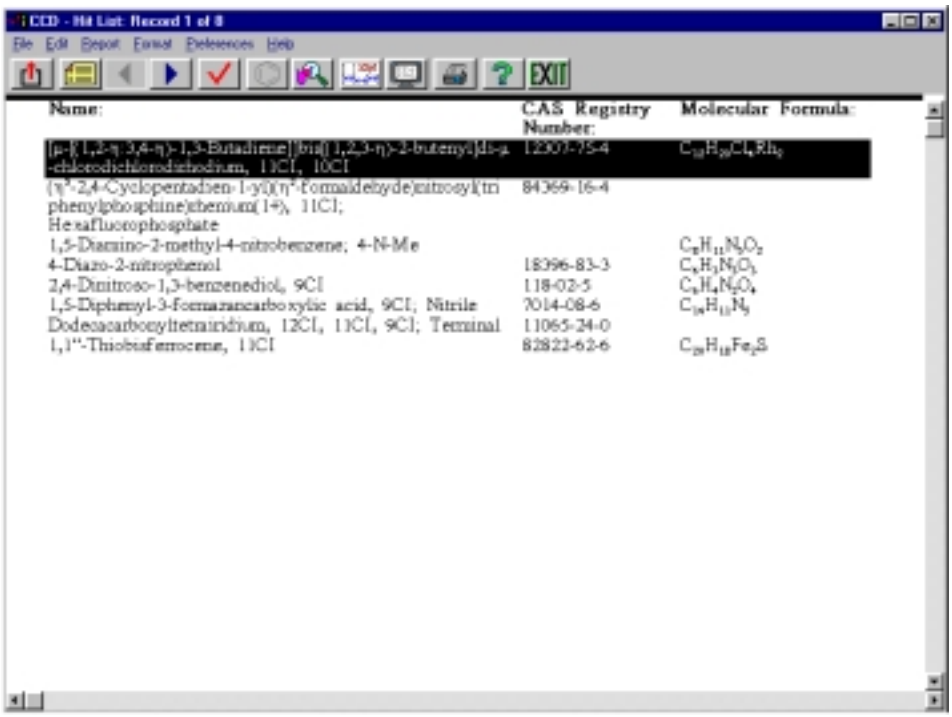


Fig.11: The Hitlist

Examining the search results

The results are displayed as a summary list of hits, giving the names of the compounds, CAS Registry numbers and molecular formulae. The first compound in the summary list is highlighted. The following icons appear at the top of the summary display:

 Refine search

 View hitlist

 Next record

 Previous record

 Bookmark/Unmark

 Structure Drawing

 Report Settings

 Display Report

 Print records

 On-screen help

 Exit

You can mark any of the hits, by selecting the hit, then clicking on the **Bookmark** icon  . A red chevron is displayed to the left of the entry. To remove the mark, highlight the entry again, then click on the **Bookmark** icon.

Additionally, the hitlist can be viewed and printed in a variety of customisable report formats (see below).

Displaying the entry

To display any entry, simply highlight the required hit and double click on it.

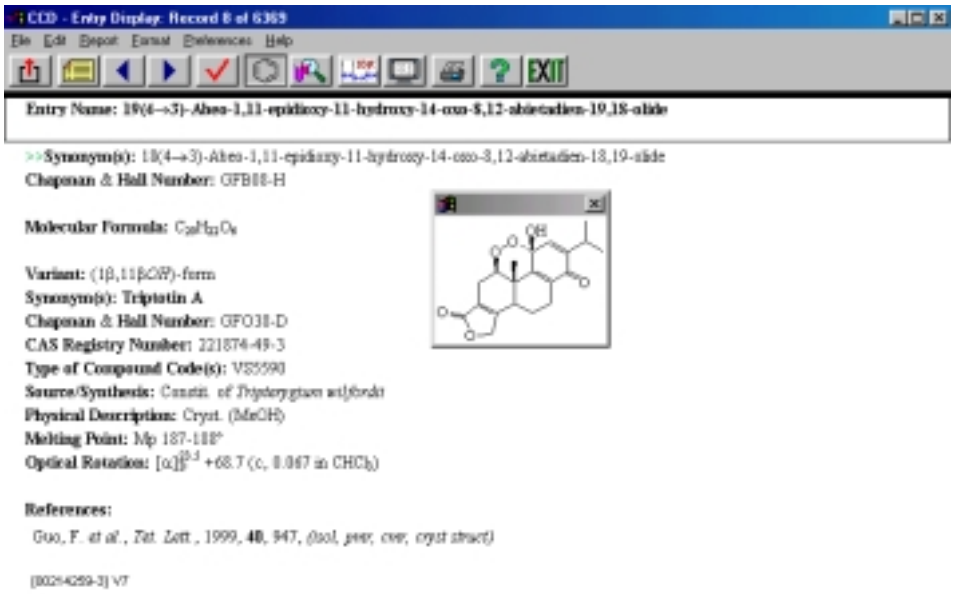


Fig.12: Typical entry

A typical entry is shown above. Structure display may be switched off (see below).

Cross references to related compounds are indicated by a blue 'hot spot'. Simply position your mouse pointer over this and the cursor will change to a hand shape. Click once and you will be taken to the cross referenced entry.

Hazard and toxicity information is displayed in red.

You can mark or unmark the entry by clicking on the **Bookmark** icon  .

Display format

You can change the display of the entry using the options in the **Format** menu:

Option	*What is displayed*
Full Fielded	The complete entry, but in a fielded layout with field titles
Standard	The complete entry as it would appear in the printed work

The default field setting is the **Full Fielded** display but this is customisable using the **Format** menu.

Viewing structures

Click on the **Structure** icon  to display a structure. To switch off the structure display, click again on the icon. The structure will appear in a box that can be moved around the screen to the desired position.

For the main entry compound the structure will show stereochemistry and numbering systems where relevant. For a variant or a derivative compound (e.g. Et ester, oxime), the structure is derived from a 2-D connection table and does not contain stereochemical information.

To display the structure of a particular compound, click on the **Structure** icon and then click on the name of the compound in question. The selected compound is highlighted in green, and the structure appears in a separate box as shown:

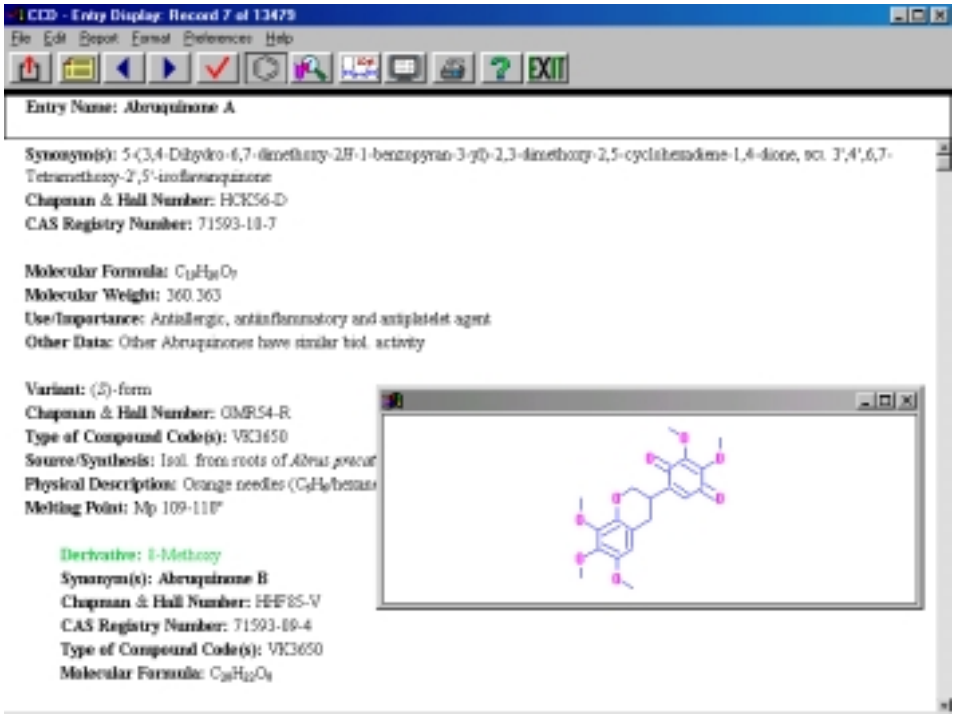


Fig.13: Entry display showing structure display for derivatives

Transferring structure to structure drawing screen

If you wish to use a structure as your query in structure drawing, simply click on the  icon. The structure drawing screen appears showing the chosen structure (see Fig. 14), which can then be modified according to need. Once modification is complete, click on the **green arrow** to return to compound search and perform your search.

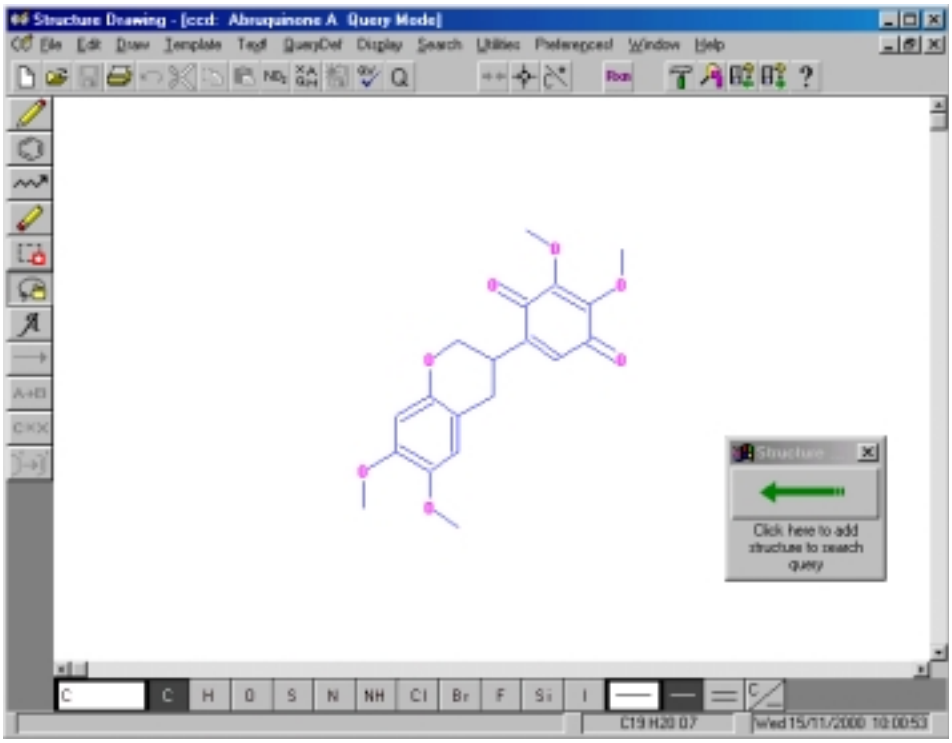


Fig. 14: Tranferring structure to structure drawing screen

Exporting text and diagrams

Both the text and the diagram may be transferred to the clipboard for export, for example to word processing packages. To copy the entry to the clipboard, click on the **Edit** menu and choose **Select All**. To copy the text, choose **Copy Text** from the **Edit** menu. To copy the diagram, choose **Copy Image** from the **Edit** menu. **Note** that you must switch on structure display, by clicking on  , in order for **Copy Image** to become active.

Printing the entry

You can print entries either from the hitlist or from the entry display. Click on the **Print Records** icon  and you will be prompted to choose All Records, Current Record or a range of records. Select the appropriate print option and click **OK**.

As default both the text and the main entry structure will be printed out. If you want to print the text only (or the structure only) click on **Preferences** menu item and deselect the appropriate item. Note that structures for the variant and derivative compounds will not be printed out.

Printing the hitlist

To print the hitlist (Name, CAS Registry No. and Molecular Formula) click on the **File** menu, then **Print Hit List**. You will be prompted to choose All Rows, Current Row or a range of rows. Select the appropriate print option and click on **OK**.

Additionally the hitlist can be viewed and printed in a variety of customisable report formats (see below).

Customising display and printing options

You may display and print the hitlist in a variety of formats, including whichever fields you like, and in any order. **Note** that the structures displayed in the report format do not show the stereochemical information as viewed in the entries.

To view the current report settings click on the **Display Report** icon  :

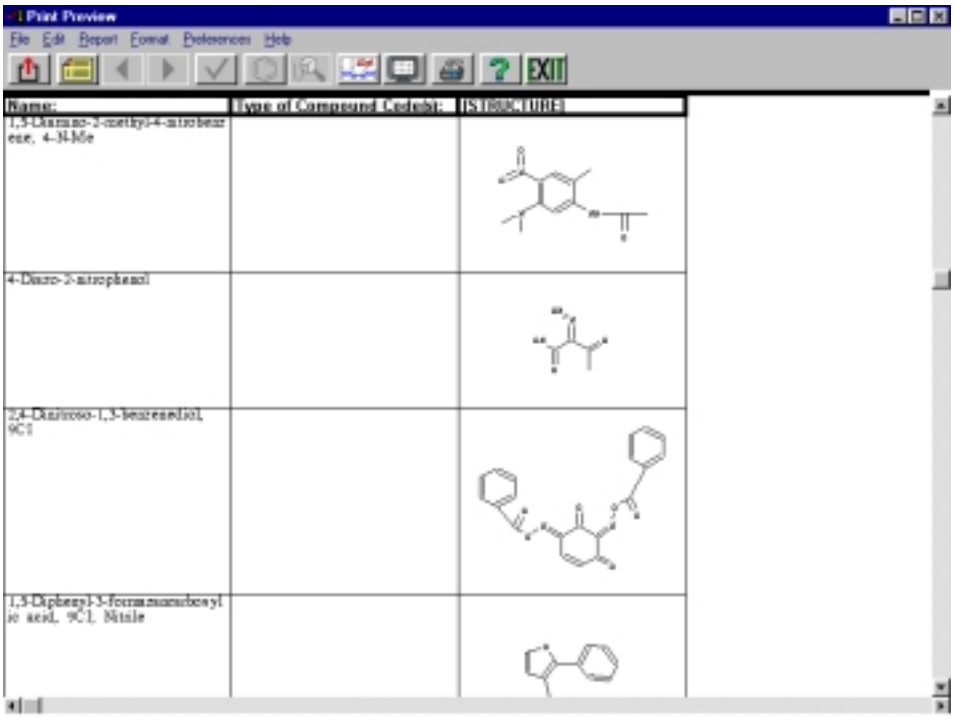


Fig. 15: Display report

The default report shows Name and Structure only, but you may change both the fields displayed and the order they are displayed in.

Click on the **Report Settings** icon  and you will be presented with a dialog box:

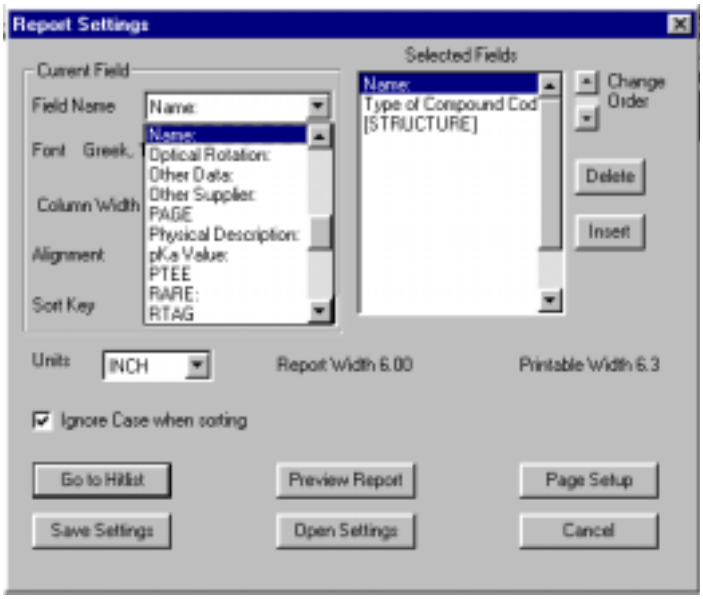


Fig. 16: Report Settings

- To **change** a field – click on the field you wish to change in the **Selected Fields** box, then select the field you require from the list of field names.
- To **add** a field – click on the empty line below the last field in the **Selected Fields** box, then select the field you require from the list of field names.
- To **remove** a field – click on the unwanted field from the **Selected Fields** box, then click on **Delete**.
- To change the order in which the fields appear within the report, select the field you wish to move, then click on the **Change Order** scroll bar to move this field up or down.
- To change the sort order (the default is alphabetical on title name) e.g. to sort on melting point, click on the Melting Point field in the **Selected Fields** box, then click on **Sort key**. You may choose from ascending or descending. You can choose to sort on two fields, one as a primary sort key and one as a secondary sort key.
- To **save** a particular report format - click on **Save Settings** and you will be prompted to save the current settings with a filename.
- To **revert** to a particular report format - click on **Open Settings** and open the relevant report.
- To **view** the resulting report - click on **Preview Report**.
- To **print** the resulting report - click on **Report** and then select the items to be printed.

Additional structure search features

The following features are available within the structure searching programs, but are not described in this manual. Please consult the online **Help** screens.

- Detailed use of drawing shortcuts
- Drawing fused ring systems
- Adding text to a structure
- Drawing generic structures
- Drawing variable points of attachment
- Drawing repeating groups, square brackets and multipliers
- Different methods of displaying structures, e.g. changing the display of the carbon atoms, showing variable points of attachment, etc.
- Adding structural attributes, such as charges, abnormal valencies

List of icons

Compound Search


Back to previous screen


Run search


View hitlist


Edit search form


Special symbol keypad


Operator toolbox


Clear terms


Combine hitsets


Show search history


Open strategy


Save strategy


Help

Exit program


Change direction of search


Browse index

Additional Icons used in hitlist/entry display


Previous record


Next record


Bookmark/unmark entry


Show diagram


Structure drawing

Report settings


Preview report


Print records

Icons on the structure drawing screen

	New	Start a new structure
	Print	Print the current structure
	Undo	Undo the last action
	Cut	Cut the selected area to the clipboard
	Copy	Copy the selected area to the clipboard
	Paste	Paste clipboard contents into the current structure
	Shortcut	Select a shortcut
	Variable	Select a variable
	Query Verify	Verify query attributes on a node or bond
	Preferences	Structure drawing and chemical preferences
	Fuse	Fuse two fragments together
	Centre	Centre the structure in the drawing window
	Carbons	Change display of carbon atoms (dot, C or angle)
	Reaction	Toggle display of reaction data
	Start Search	Start search for current structure
	Save Query	Save a query file
	Open Query	Open a query file
	Help	Show structure drawing help

The drawing palette

Pencil Tool

Ring Tool

Chain Tool

Eraser Tool

Selection Tool

Lasso Tool

Text Tool

Reaction Arrow Tool - *not used in this application*

Reaction Role Tool - *not used in this application*

Reaction Site - *not used in this application*

Reaction Mapping Tool - *not used in this application*